The Virtual Element Method for transport simulations in Discrete Fracture Networks

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**Project title**  Metodo degli Elementi Virtuali applicato alla simulazione di flussi in reti discrete di fratture

**Funds**  1200 €

Outline

1 **Discrete Fracture Networks**
   - Domain
   - Continuous model

2 **The Virtual Element Method for transport equations on DFN**
   - Functional spaces
   - SUPG stabilized discrete problem
   - Local orthogonal polynomials in VEM
   - A posteriori error estimation for VEM

3 **Summary of results**
Mesh generation issues

The generation of triangular meshes conforming to intersections is impossible in many practical situations.

Figure: An example of Discrete Fracture Network (DFN)
Polygonal meshes on Discrete Fracture Networks

Mesh generation issues

The generation of triangular meshes conforming to intersections is **impossible** in many practical situations.

Locally conforming polygonal meshes

Starting from an **independent** triangular mesh on each fracture, **cut triangles** at the intersections.
## Polygonal meshes on Discrete Fracture Networks

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<td>Build locally conforming meshes, then <strong>add nodes</strong> to both discretizations in such a way that the resulting induced discretizations are the same.</td>
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Advection-diffusion-reaction equations on DFN

- **Local variational problems**: \( \forall i \in \mathcal{I}, \) find \( u_i \in V_i := H^1_{0,\Gamma_{D,i}}(F_i) \) such that, \( \forall v_i \in V_i, \)

\[
(\mu_i \nabla u_i, \nabla v_i)_{F_i} + (\beta_i \cdot \nabla u_i, v_i)_{F_i} + (\gamma_i u_i, v_i) = \mathcal{F}_i(v_i) \\
+ \sum_{m \in \mathcal{M}_i} \left\langle \left[ \mu \nabla u_i \cdot \mathbf{n}_m^i \right]_{\Gamma_m}, \gamma_{\Gamma_m}(v_i) \right\rangle_{\Gamma_m},
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Advection-diffusion-reaction equations on DFN

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\[
(\mu_i \nabla u_i, \nabla v_i)_{F_i} + (\beta_i \cdot \nabla u_i, v_i)_{F_i} + (\gamma_i u_i, v_i) = F_i(v_i) \\
+ \sum_{m \in \mathcal{M}_i} \left\langle \left[ \mu \nabla u_i \cdot \hat{n}^i_m \right]_{\Gamma_m}, \gamma_{\Gamma_m}(v_i) \right\rangle_{\Gamma_m},
\]

- **Coupling conditions**: \( \forall m \in \mathcal{M}, \) if \( \Gamma_m = F_i \cap F_j, \)

\[
[u]_{\Gamma_m} = \gamma_{\Gamma_m}(u_i) - \gamma_{\Gamma_m}(u_j) = 0, \\
\left[ \mu \nabla u_i \cdot \hat{n}^i_m \right]_{\Gamma_m} + \left[ \mu \nabla u_j \cdot \hat{n}^j_m \right]_{\Gamma_m} = 0.
\]
A formulation ready for domain decomposition

Let $\mathcal{B}: V \times V \to \mathbb{R}$ such that

$$\mathcal{B}(u, v) := \sum_{i \in I} (\mu_i \nabla u_i, \nabla v_i)_{F_i} + (\beta_i \cdot \nabla u_i, v_i)_{F_i} + (\gamma_i u_i, v_i)_{F_i}$$

Then there exist a unique $(u, \lambda) = V \times M := \prod_{m \in \mathcal{M}} H^{-\frac{1}{2}}(\Gamma_m)$ solution of

$$\begin{cases} \mathcal{B}(u, v) + b^M(v, \lambda) = F(v) & \forall v \in V \\ b^M(u, \psi) = 0 & \forall \psi \in M \end{cases}$$

where

$$b^M(v, \psi) = \sum_{m \in \mathcal{M}} \left\langle \psi_m, \llbracket v \rrbracket_{\Gamma_m} \right\rangle_{\Gamma_m}.$$
Virtual Element Space of order $k$

**$H^1$-orthogonal projection**

Let $\Pi_k^\nabla : H^1 (E) \rightarrow \mathbb{P}_k (E)$ be such that

$$(\nabla (v - \Pi_k^\nabla v), \nabla p)_E = 0, \forall p \in \mathbb{P}_k (E)$$

and

$$\begin{cases} (\Pi_k^\nabla v, 1)_{\partial E} = (v, 1)_{\partial E} & \text{if } k = 1 \\ (\Pi_k^\nabla v, 1)_E = (v, 1)_E & \text{if } k \geq 1 \end{cases}$$
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**Local VEM space**

$$V^E_\delta := \{ v \in H^1(E) : \Delta v \in P_k(E), \gamma_e(v) \in P_k(e), \forall e \subset \partial E, \gamma_{\partial E}(v) \in C^0(\partial E), (v, p)_E = (\Pi_k^\nabla v, p)_E, \forall p \in P_k(E)/P_{k-2}(E) \}.$$
### Degrees of freedom

- the values at the vertices of the polygon;
- if $k \geq 2$, for each edge $e \subset \partial E$, the value of $v_{\delta}$ at $k - 1$ internal points of $e$;
- if $k \geq 2$, local moments with respect to polynomials of order $\leq k - 2$.

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<th>DOFs for $k = 2$</th>
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<td><img src="image.png" alt="Polygon with DOFs" /></td>
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Computability

Basis functions are not known analytically inside polygons. Using the d.o.f. we can compute polynomial projections of the functions and their gradients.
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Computability

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Global spaces

$$V_{\delta,i} = \left\{ v \in C^0(F_i) : v \in V^E_\delta \forall E \in T_{\delta,i} \right\}, \quad V_\delta = \prod_{i \in \mathcal{I}} V_{\delta,i}.$$
**SUPG-stabilized VEM**

Let $\mu_E = \|\mu\|_{L^\infty(E)}$, $\beta_E = \|\beta\|_{L^\infty(E)}$, $\gamma_E = \|\gamma\|_{L^\infty(E)}$. We define

$$B_{\text{supg}, \delta}(u_\delta, v_\delta) = \sum_{E \in T_\delta} a^E_\delta(u_\delta, v_\delta) + b^E_\delta(u_\delta, v_\delta) + c^E_\delta(u_\delta, v_\delta) + d^E_\delta(u_\delta, v_\delta),$$

where

$$a^E_\delta(u_\delta, v_\delta) = \left(\mu \Pi_{k-1}^0 \nabla u_\delta, \Pi_{k-1}^0 \nabla v_\delta \right)_E + \tau_E \left(\beta \cdot \Pi_{k-1}^0 \nabla u_\delta, \beta \cdot \Pi_{k-1}^0 \nabla v_\delta \right)_E$$

$$+ \left(\mu_E + \tau_E \beta^2 E \right) S^E \left((I - \Pi^\nabla_k) u_\delta, (I - \Pi^\nabla_k) v_\delta \right),$$

$$b^E_\delta(u_\delta, v_\delta) = \left(\beta \cdot \Pi_{k-1}^0 \nabla u_\delta, \Pi_{k-1}^0 v_\delta \right)_E,$$

$$c^E_\delta(u_\delta, v_\delta) = \left(\gamma \Pi_{k-1}^0 w_\delta, \Pi_{k-1}^0 v_\delta + \tau_E \beta \cdot \Pi_{k-1}^0 \nabla v_\delta \right)_E,$$

$$d^E_\delta(u_\delta, v_\delta) = \left(-\nabla \cdot \left(\mu \Pi_{k-1}^0 \nabla u_\delta\right), \tau_E \beta \cdot \Pi_{k-1}^0 \nabla v_\delta \right)_E,$$

$$F^E_{\text{supg}, \delta}(v_\delta) = \left(f, \Pi_{k-1}^0 v_\delta + \tau_E \beta \cdot \Pi_{k-1}^0 \nabla v_\delta \right)_E,$$

$$\tau_E = \min \left\{ \frac{\tilde{C}_k h^2_E}{\mu_E}, \frac{h_E}{2\beta_E}, \frac{1}{2\gamma_E} \right\}.$$
A priori error estimate for VEM-SUPG formulation

Assumption

Suppose local extra-regularity of VEM functions, i.e. \( \exists r > 0 \) independent of \( \delta \) such that \( r \leq k \) and \( V_\delta^E \subseteq H^{r+1}(E) \), \( \forall E \in \mathcal{T}_\delta \).
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**Errore measure**

\[
\| \mathbf{v} \|_{\mu, \beta, \gamma}^2 = \sum_{E \in T_\delta} \left( \| \sqrt{\mu} \nabla \mathbf{v} \|_E^2 + \tau_E \| \beta \cdot \nabla \mathbf{v} \|_E^2 + \| \sqrt{\gamma} \mathbf{v} \|_E^2 \right)
\]
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Errore measure
\[
\| v \|_{\mu \beta \gamma}^2 = \sum_{E \in T_\delta} \left( \| \sqrt{\mu} \nabla v \|_E^2 + \tau_E \| \beta \cdot \nabla v \|_E^2 + \| \sqrt{\gamma} v \|_E^2 \right)
\]

Theorem
If \( u \in H^{s+1}(\Omega) \) is the exact solution and \( u_\delta \) the discrete VEM solution, and if the problem coefficients are sufficiently regular, it holds
\[
\| u - u_\delta \|_{\mu \beta \gamma} \leq C \max_{E \in T_\delta} \left\{ \sqrt{\mu}_E, \sqrt{h_E \beta_E}, h_E \sqrt{\gamma}_E \right\} h^s \| u \|_{s+1} + o(h^s) \left( \| u \|_{s+1} + \| f \|_{s-1} \right).
\]
Discrete problem

Choose a finite dimensional space \( M_\delta \subset M \) containing constants on each trace.
Find \( u_\delta \in V_\delta, \lambda_\delta \in M_\delta \) such that

\[
\begin{align*}
B_{\text{supg},\delta}(u_\delta, v_\delta) + b^M(v_\delta, \lambda_\delta) &= F_{\text{supg},\delta}(v_\delta) \quad \forall v_\delta \in V_\delta \\
b^M(u_\delta, \psi_\delta) &= 0 \quad \forall \psi_\delta \in M_\delta
\end{align*}
\]
Choose a finite dimensional space $M_\delta \subset M$ containing constants on each trace.

Find $u_\delta \in V_\delta$, $\lambda_\delta \in M_\delta$ such that

\[
\begin{aligned}
B_{\text{supg},\delta}(u_\delta, v_\delta) + b^M(v_\delta, \lambda_\delta) &= \mathcal{F}_{\text{supg},\delta}(v_\delta) & \forall v_\delta \in V_\delta \\
 b^M(u_\delta, \psi_\delta) &= 0 & \forall \psi_\delta \in M_\delta
\end{aligned}
\]

**Computability**

Coupling terms are computable since polygon edges are conforming to traces.
Possible approaches

Locally conforming mesh

Mortar approach to impose weak continuity at traces. Lagrange multipliers are piecewise polynomial functions.
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Locally conforming mesh

Mortar approach to impose **weak continuity** at traces. Lagrange multipliers are piecewise polynomial functions.

Globally conforming mesh

Impose **strong continuity**. Lagrange multipliers are the “dofs” operators.

\[ \forall k \in \{1, \ldots, N_m\}, \quad u_{\delta i}(x^m_k) = u_{\delta j}(x^m_k). \]
Mixed VEM in Discrete Fracture Networks

The same framework is ready for the application of Mixed Virtual Elements. Globally conforming meshes allow us to obtain velocity fields that are exactly balanced at intersections.

**Figure:** Velocity field
Mixed VEM in Discrete Fracture Networks

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**Figure:** Velocity field

**Computational framework for real life simulations**

1. Solve a pure diffusion equation in mixed form for the pressure field, obtaining the Darcy velocity;
2. Using the Darcy velocity, simulate transport of contaminants or geothermal systems.
Using orthogonal polynomials on badly shaped polygons

**Figure:** Instabilities with high order VEM on badly shaped polygons

(a) Order 1

(b) Order 3

(c) Order 4

**Proposed strategy**

Solve a *local eigenvalue problem only on badly shaped polygons* to orthogonalize the polynomial basis used for computing polynomial projections.
A posteriori error estimates

Objective

Consider a pure diffusion second order linear PDE. We want to find a computable, local error estimator $\eta_{R,E}$, $\forall E \in T_\delta$, such that

$$\sum_{E \in T_\delta} \eta_{R,E}^2 \lesssim \| \sqrt{\mu} \nabla (u - u_\delta) \|^2 \lesssim \sum_{E \in T_\delta} \eta_{R,E}^2.$$
A posteriori error estimates

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Consider a pure diffusion second order linear PDE. We want to find a computable, local error estimator $\eta_{R,E}$, $\forall E \in \mathcal{T}_\delta$, such that

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Computability

Define the following post-processing of the discrete solution $u_\delta \mapsto u_\delta^{\pi} \in \mathbb{P}_k(\mathcal{T}_\delta)$, such that, $\forall E \in \mathcal{T}_\delta$,

$$\begin{cases} 
(\mu \nabla u_\delta^{\pi}, \nabla p)_E = (\mu \Pi^{0}_{k-1} \nabla u_\delta, \nabla p)_E & \forall p \in \mathbb{P}_k(E), \\
(u_\delta^{\pi}, 1)_{\partial E} = (u_\delta, 1)_{\partial E} .
\end{cases}$$
Theorem

Suppose $\mu$ is piecewise constant and there exists a stable linear operator $I_\delta : V_\delta \rightarrow W_\delta := \{ \nu_\delta \in V_\delta : S((I - \Pi_k^\nabla) u_\delta, (I - \Pi_k^\nabla) \nu_\delta) = 0 \}$. Define

$$\eta_{R,E}^2 := \frac{h_E^2}{\mu_E} \| f_\delta + \nabla \cdot (\mu \nabla u_\delta^\pi) \|_E^2 + \frac{1}{2} \sum_{e \in \mathcal{E}_\delta \cap \partial E} \frac{h_e}{\mu_e} \| [\mu \nabla u_\delta^\pi \cdot \hat{n}]_e \|_e^2.$$

Then,

$$\sum_{E \in T_\delta} \eta_{R,E}^2 \lesssim \sum_{E \in T_\delta} \| \sqrt{\mu} \nabla (u - u_\delta^\pi) \|_E^2 \lesssim \sum_{E \in T_\delta} \eta_{R,E}^2.$$

The existence of the operator $I_\delta$ can be easily proved for $k > 1$. For $k = 1$, a possible proof can be devised relying on very weak assumptions on the mesh.
Summary of results

- A complete framework for the simulation of transport phenomena in Discrete Fracture Network is devised.

- Primal and mixed Virtual Element Methods are a crucial ingredient for using polygonal meshes, allowing to impose strong or weak continuity / balance of fluxes.

- SUPG stabilized VEM are introduced in order to deal with advection dominated problems (very good numerical results even with $\text{Pe} \sim 10^{11}$).

- A strategy based on local orthogonal polynomials is proposed to deal with instabilities arising with high order VEM on badly shaped polygons.

- A posteriori error estimation is possible for the Laplace equation, allowing for adaptivity.
References


